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13. ABSTRACT (Maximum 200 words)

When a fluid flow is composed of several gas species having different molecular weights and molecular composition, such as air, in particular at high temperature, various nonequilibrium effects lead to well-known changes in the flow structure over that for a simple gas. These are frequently termed relaxation effects when associated with nonequilibrium of the vibrational modes of a polyatomic molecule, chemical composition of a dissociating molecule, or degree of ionization of an ion. Relaxation effects also arise owing to a difference in the molecular weights of two species making up a flow, which introduces a time lag in the transfer of translational energy between the two. If the time scale of the relaxation phenomenon is very short when compared

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Final Report

for the Period

September 1, 1993 to August 31, 1996

on

DAMPING IN RAREFIED NONSTEADY FLOWS
(AASERT FY93)

Grant No. F49620-93-1-0542

by the

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Stanford University, Stanford, California 94305

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December 20, 1996

I. Introduction

This final report is a summary of work carried out under Grant No. F49620-93-1-0542 (AASERT Award) during the period September 1, 1993 to August 31, 1996.

When a fluid flow is composed of several gas species having different molecular weights and molecular composition, such as air, in particular at high temperature, various nonequilibrium effects lead to well-known changes in the flow structure over that for a simple gas. These are frequently termed relaxation effects when associated with nonequilibrium of the vibrational modes of a polyatomic molecule, chemical composition of a dissociating molecule, or degree of ionization of an ion. Relaxation effects also arise owing to a difference in the molecular weights of two species making up a flow, which introduces a time lag in the transfer of translational energy between the two. If the time scale of the relaxation phenomenon is very short when compared with the time scale of the flow, then one is permitted to model the process as a frequency-dependent damping thereby greatly simplifying the set of equations used in theoretical studies. When the time scale of the relaxation phenomenon is comparable to the time scale of the flow, then one must employ individual rate equations for the different relaxation processes and the resulting equation set is much more complex. Clearly, the greatest knowledge is gained if one is able to study the entire range of relative time scales. The effect of mass disparity has been the least studied in the above group, principally because of a lack of suitable experimental information. However, the effect of mass disparity is very important in a numerical scheme for simulating rarefied flows called the direct simulation Monte Carlo method when it is used to model a chemically reacting flow involving a number of different species. An important need is to establish how one models binary collisions at the molecular level between two species having different masses. This involves both a determination of the relevant molecular constants used in the modeling and a clear understanding of the relevant physics, both at the microscale of individual collision and the macroscale of gas dynamic flow processes.

The goal of this study is to determine the validity of the models, molecular data, and assumptions used in the standard implementation of the Direct Simulation Monte Carlo (DSMC) method for simulating multiple-species flows. Of primary concern

is the manner in which collisions between non-identical species are handled. This work is motivated by a desire to obtain physically realistic predictions of flows which may be sensitive to the details of collision processes, e.g., the chemically reacting flow about a hypersonic vehicle on reentry into the earth's atmosphere. Typically these high enthalpy flows consist of many species, some having relatively disparate physical properties such as mass and/or diameter. The accurate prediction of flow characteristics defining heat transfer and drag on the body is intimately connected to the correct modeling of collisions between these non- identical species.

The basic elements of the DSMC collision model that are in question are the use of:

(1) power-law intermolecular potentials for the forces between interacting molecules;

(2) readily available transport data for single-species gases to arrive at collision parameters defining binary collisions between like species; and

(3) an ad hoc combining rule for single-species data to specify parameters needed to perform binary collisions between non-identical species.

The appropriateness of each of these elements is addressed by comparing simulations of an unsteady, one-dimensional flow in a binary mixture of disparate gases to existing experimental data.

A summary of the findings is provided here. A detailed account of this work will appear in the Ph.D. thesis by S. T. Whitlock [1]. Results of this work have been presented by Whitlock and Baganoff in [2] and [3] and will appear in [4].

II. Experimental Data

The experimental data available are in the form of wall-pressure histories resulting from the reflection, from an isothermal wall, of a shock wave in a mixture of helium (He) and xenon (Xe). The experimental data were obtained roughly 30 years ago by Baganoff at Caltech concurrently with data reported in [5].

Data are available for a range of Xe concentrations from approximately 1% (by number density) to roughly 8%. In addition, data for pure He and pure Xe flows are available. The experimental data for all cases except the pure Xe flow are displayed

in Figure 1. In each case, the incident shock Mach number based on the He speed of sound is about 2.7. This sets the Mach number based on Xe speed of sound in the pure Xe flow to roughly 15. The pressure of the test gas is 0.5 mm Hg for all cases except the pure Xe flow. In this case, the pressure of the test gas is 0.1 mm Hg.

Due to the one-dimensional nature of this flow and the fact that He and Xe are monatomic gases devoid of internal structure, this binary-gas normal shock wave is perhaps the simplest flow with substantial departures from equilibrium from which to gain insight into the details of collision processes. Furthermore, this flow is dominated by He-Xe collisions, so it is ideal for the study of collisions between non-identical species. A quantitative measure of the validity of the DSMC collision model is obtained from a comparison of the simulated and experimental relaxation times for the reflection process. The molecular weight and diameter of He:Xe are sufficiently disparate (1:33 and 1:2, respectively) so that relevant time scales of the reflection process are distinct.

Simulations of this unsteady flow are not trivial to obtain. Historically, time-dependent problems, such as the unsteady flow of interest here, have been too computationally intensive to perform. However, recent advances in the size and speed of parallel supercomputers have made many problems that were once intractable now more feasible. In particular, by porting a version of our particle method code to the Intel Paragon parallel supercomputer (see [6]), we have the resources to realistically simulate certain unsteady flows. An important offshoot of this work is the opportunity to gain experience implementing an unsteady DSMC code on a parallel computer. The result of this experience, a strategy for simulating this unsteady flow, is presented in the next section.

III. Simulation Strategy

A two-step simulation strategy is adopted to simulate this flow in a most cost-effective manner. In the first step, the incident shock profile is computed. This step is performed in the incident-shock-fixed frame so that the flow reduces to steady state. As a result, time averaging can be used to produce statistically smooth profiles. An example of the density profiles for a 97% He - 3% Xe (by number density) flow are

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shown in Figure 2. Note how the He "leads" the Xe in formation of the incident wave. Similar behavior is reported by Bird [7].

In the second step, the steady state profile obtained from state one is used as an initial condition to the unsteady flow of interest here. In this case, the simulation is performed in the lab-fixed frame so that the incident shock moves toward the wall. Eventually, the wave encounters the wall and reflects from it. Because the incident profile is saved as a result of step one, the second step may be repeated numerous times, each time appropriately using a different seed for the random number generator. The resulting data can then be ensemble averaged to produce cleaner time-dependent profiles.

IV. Elements of DSMC Model

To compare simulations to the experimental data, it is essential to establish a relationship between the simulation and physical domains. In the standard implementation of the method, it is assumed that, at least for the range of temperatures commonly encountered in DSMC applications, the intermolecular forces between particles are purely repulsive. As a result, the intermolecular potential, V, can be expressed as a power law in separation distance, r, as

$$V = \frac{A}{r^\alpha}.$$ (1)

Doing so leads to a power-law relationship for the transport properties of the gas of the form

$$\mu \sim T^{\frac{1}{2} + \frac{2}{\alpha}}.$$ (2)

Here, μ and T are the viscosity and temperature of the gas and α is the power-law exponent appearing in the expression for the intermolecular potential. By fitting this assumed functional form to actual data, the value for the power-law exponent and hence the variation of the molecular collision diameter with temperature may be determined. (The collision diameter may be related to the viscosity of the gas as described by Chapman and Cowling [8].) A reference collision diameter may be obtained from the viscosity of the gas for some specified reference temperature.

A fundamental assertion in the standard implementation of the DSMC method is that a flow may be accurately simulated once the reference collision diameter and

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power-law exponent for each class of collision occurring in the flow are known. Furthermore, it is assumed that the reference diameters and power-law exponents describing collisions between non-identical species may be defined by a simple combination of the single-species data. Usually, the inter-species parameters are taken to be the simple arithmetic average of the single-species data, namely,

$$d_{i-j} = \frac{1}{2}(d_{i-i} + d_{j-j}) \qquad (3a)$$

$$\alpha_{i-j} = \frac{1}{2}(\alpha_{i-i} + \alpha_{j-j}). \qquad (3b)$$

Here, d_{i-j} and α_{i-j} are the reference collision diameter and power-law exponent for collisions between particles of type i and j.

	He-He	Xe-Xe	He-Xe
d_{ref}	2.33	5.74	4.04
α	12.5	5.71	9.11

Table 1. Collision parameters for a flow in He and Xe due to Chapman and Cowling [8].

Typical values of the collision parameters appropriate for a flow in a binary mixture of He and Xe obtained from Chapman and Cowling [8] are displayed in Table 1. The arithmetic average combining rule is used to define collision parameters for the He-Xe class of collisions.

V. Validation of the Method for Single-Species Flows

Simulations of the wall-pressure histories resulting from the reflection of shock waves in pure He and pure Xe are compared to experiment in Figure 3. The physical data used for the reference diameters and power-law exponents are those displayed in Table 1. Note the excellent agreement between simulation and experiment for the pure He flow. The simulation is observed to capture not only the correct translational relaxation time, but also the gradual thermal relaxation due to the thermal boundary layer adjacent to the cold end wall.

The agreement for the pure Xe flow is not as impressive. However, for this flow, the incident shock Mach number is roughly 15. This leads to a post-reflection

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temperature of approximately 38,000K so that it is likely that the flow is partially ionized. Currently, our particle method code does not allow for such physical effects. Note also that the experimental data terminate roughly 4 microseconds into the test. This occurred due to failure of the pressure gauge. Owing to the extreme conditions of this flow, the agreement shown is accceptable.

The favorable agreement between simulated and experimental relaxation times for these two cases suggests that at least part of the DSMC collision model is working properly. The agreement confirms that the use of a power-law intermolecular potential is reasonable, at least for flows of single-species gases. What the agreement does **not** reveal, in addition to any insight into the validity of the arithmetic average combining rule, is any significant information about the suitability of the data used to define the single-species collision parameters. This is because the DSMC binary collision model is a function of the relative size of colliding particles. In a flow of a single-species gas, the relative diameter is necessarily unity. Thus, the only parameter affecting the flow is the power-law exponent. Previous studies (see, e.g., [7]) have shown that flows are relatively insensitive to the exact value of the power-law exponent provided that it is somewhat realistic.

VI. Application of the Standard Approach to Binary Mixtures

The result of a more revealing test, one which addresses all three elements of the DSMC collision model, is given in Figure 4. Here, the simulation of the reflection process in a mixture composed of 92.3% He and 7.7% Xe is compared to experiment. This simulation was done using the collision parameter data given in Table 1. An examination of the figure shows that the simulation predicts a significantly shorter relaxation time than the experiment gives.

The failure of the DSMC simulation to give a more realistic prediction of the relaxation time is due to a He-Xe collision diameter which is too large. The exact cause for this is unclear. Whether the He-Xe diameter is too large due to fault of the simple combining rule or the single-species data used as input to the combining rule is unknown. Clearly, however, one or both of these elements of the standard model is in error.

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VII. Improved Intermolecular Potential

The two elements of the DSMC collision model in question, namely, the single-species data and the use of the simple combining formula, are a direct result of the assumption of a power-law intermolecular potential. Thus, in order to discover the source of the deficiencies in the model, it was determined that a better understanding of the intermolecular potentials driving collisions in this noble gas mixture was warranted. Consultation of the chemical physics literature revealed the best characterization of the intermolecular potentials for noble gases known to date in the work of Aziz et al. (see [9- 11]). Here, researchers assumed a functional form of the Hartree-Fock-Dispersion (HFD-B) type for the potential and defined function coefficients by fitting to transport and virial coefficient data. The resulting intermolecular potentials appropriate for the collision classes in the He-Xe mixture (for the temperature range of interest) are shown in Figure 5. Power-law fits to these potentials are also plotted.

An examination of Figure 5 reveals that a power-law fit to the state-of-the-art potentials appears to be reasonable. The relevant collision parameters derived from the power-law fit to the HFD-B potential are given in Table 2. The corresponding values taken from the Chapman and Cowling data are provided for the purpose of comparison. Note that the reference collision diameters obtained from the HFD-B potentials are significantly smaller than those derived from the Chapman and Cowling data. Simulations using these new parameters are then based on an improved set of single-species data. Note also that the HFD-B potential for the He-Xe interactions is provided explicitly. Therefore, no approximate formula is required, nor is one used, to compute the He-Xe collision parameters.

	He-He		Xe-Xe		He-Xe	
	d_{ref}	α	d_{ref}	α	d_{ref}	α
Chapman & Cowling	2.33	12.5	5.74	5.71	4.04	9.11
HFD-B	2.07	7.87	3.79	14.59	3.06	9.85

Table 2. Collision parameters in a flow of He and Xe: comparison of the Chapman and Cowling data to the power-law fit of the HFD-B potential.

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Simulated wall-pressure histories for the binary-mixture flows are compared to experiment in Figure 6. In each case, the reference collision diameters and power-law exponents for the three collision classes were obtained from a power-law fit to the HFD-B potential. Favorable agreement between simulation and experiment is evident even for the 92.3% He - 7.7% Xe flow previously considered.

The x-t diagram for the reflection process in the 97% He - 3% Xe flow is shown in Figure 7. Note the formation of a high density thermal boundary layer as the high temperature portion of the incident wave encounters the cold wall. Note also, from the superposed color scale, the rise in He concentration in the incident and reflected wave fronts. This is a direct result of the "leading" of the He as seen in the density profiles in Figure 2.

The fact that the simulations were able to predict the correct relaxation times using the power-law fit to the HFD-B data indicates two things: (1) a power-law intermolecular potential is a reasonable approximation for flows in the temperature range considered; and (2) the single-species data were at least partly responsible for the disagreement between simulation and experiment shown in Figure 4. The degree to which the arithmetic average combining rule contributed to the disagreement is still unknown. This is because the issue of combining rule is avoided in this test due to the existence of the HFD-B potential function for the He-Xe interactions. A study of the influence of this aspect of the DSMC collision model is given next.

VIII. Investigation of Combining Rules

In the general case, intermolecular potentials for inter-species interactions are not explicitly known. It is therefore essential to have some sort of approximate formula to predict these potentials. On the other hand, accurate transport data for single-species gases, from which single-species potentials may be obtained, are usually available. Hence, it is convenient to develop an approximate formula for the inter-species potential which is based on the single-species data.

For the form of the power-law intermolecular potential given in Equation (1), there are only two logical choices for the approximate formula. The first is an arithmetic average of the single-species collision parameters, d_{ref} and α, as previously given in Equation (3). The second approximate rule defines the constant, A, for the

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inter-species potential as a geometric mean of the single-species constants. The relevant power-law exponent is again defined as the arithmetic mean of the single-species data. The corresponding inter-species reference collision diameter is the value of r of the approximate potential evaluated at an energy consistent with the reference temperature.

The values for the He-Xe collision parameters computed using the HFD-B single-species data as input to the two combining rules are given in Table 3. The original parameters obtained from the Chapman and Cowling data and the power-law fit to the HFD-B He-Xe potential are provided for comparison. A graphical representation of the various He-Xe potentials is given in Figure 8. The potential for He-He collisions and the Xe-Xe reference diameter from the HFD-B data are provided as points of reference. As can be seen, the approximate potentials do respectable jobs of imitating the true He-Xe potential whereas the arithmetic average of the Chapman and Cowling data yields a potential more closely resembling that of the Xe-Xe interactions. This figure clearly suggests that the dominant factor leading to the disagreement shown in Figure 4 was the single-species data and not the approximate combining rule.

	d_{ref}	α
Chapman & Cowling	4.04	9.11
HFD-B	3.06	9.85
Arithmetic Mean	2.93	11.23
Geometric Mean	3.07	11.23

Table 3. Comparison of He-Xe collision parameters.

Simulations of the 92.3% He - 7.7% Xe flow using the various collision parameters discussed are compared to experiment in Figure 9. For display purposes, the simulation data has been smoothed using the Savitzky-Golay filtering process (see [12] for a description of the technique). An examination of this figure reveals that all of the HFD-B based data sets, including those using approximate formulas to define He-Xe collision parameters, predict the correct relaxation time. Therefore, it is concluded that the two logical choices for combining rules are appropriate provided that the single-species data used as input are physically realistic. Clearly, the single-species data reported by Chapman and Cowling are inadequate.

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IX. Conclusions

Several important conclusions about the DSMC collision model were drawn as a result of this work:

(1) for the high enthalpy flows of primary concern, a power-law intermolecular potential is a reasonable approximation;

(2) physically realistic single-species data are critical to the accurate simulation of multiple-species flows; and

(3) any logical combining rule for the approximation of inter-species collision parameters will work provided that the single-species data used as input are physically realistic.

An important offshoot of this work was the opportunity to gain some insight into the efficient implementation of an unsteady DSMC code on a parallel computer. A two-step simulation strategy was developed so that multiple occurrences of the reflection process could be obtained. This was an important accomplishment because the ensemble average of multiple runs was required in order to produce clean time-dependent results.

A more complete accounting of this work will appear in Whitlock's Ph. D. thesis [1] and will include several additional topics which are being explored in her ongoing work. These include: (1) the development of more efficient simulation strategies so that the full capabilities of the parallel computing environment may be realized; (2) the gathering of more simulated reflection occurrences for better ensemble averages; and (3) further investigation of mass related damping by the examination of He-Xe flows in the limit of a fully dispersed wave, i.e., a wave which is subsonic with respect to the He Mach number and supersonic with respect to the mixture Mach number.

Acknowledgments

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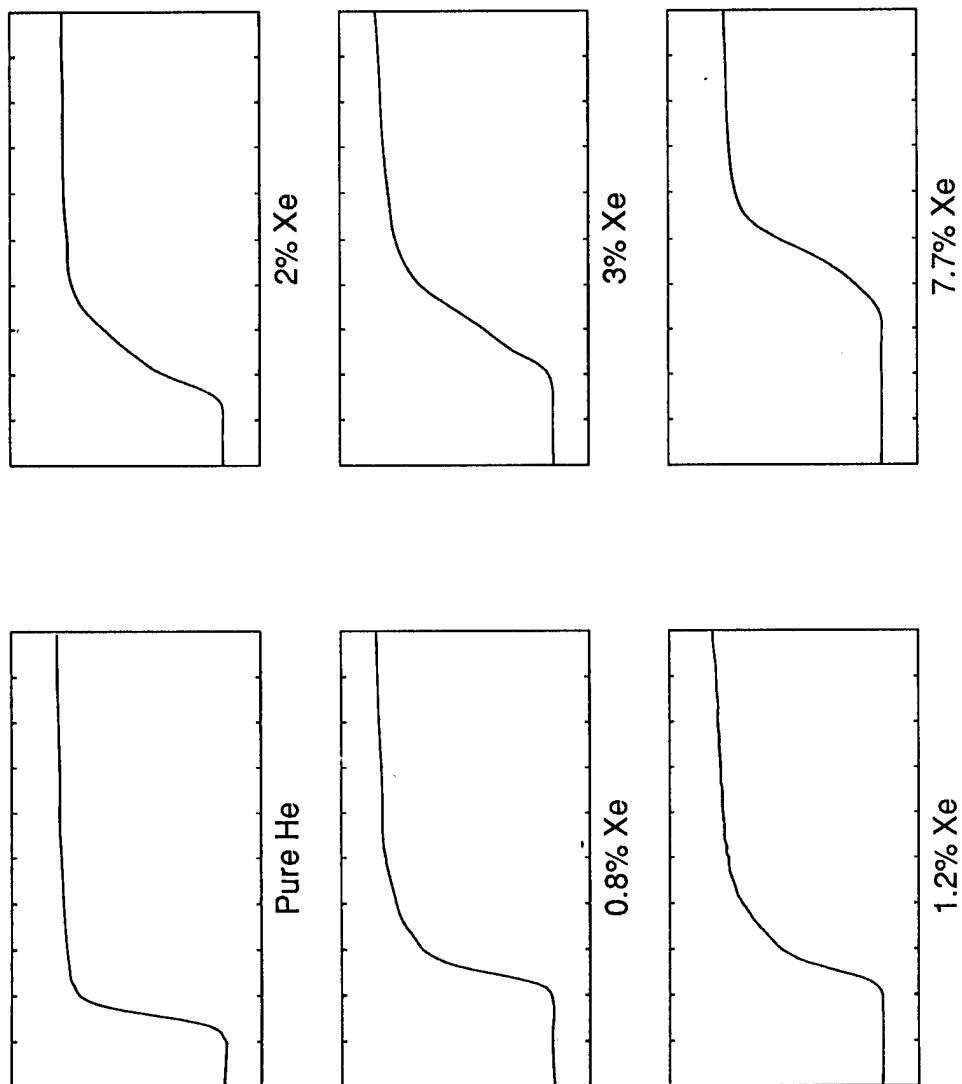
Figure 1. Available experimental data: wall pressure vs. time. The incident shock speed based on the speed of sound in He is ≈ 2.7. The sweep speed is 1 μsec/div and the upstream pressure in the mixture is 0.5mm Hg in each case.

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Figure 2. Density profiles for the incident shock in a 97% He - 3% Xe mixture. The solid line corresponds to the mass averaged mixture density. The dash and dash-dot lines represent the He and Xe concentrations respectively.
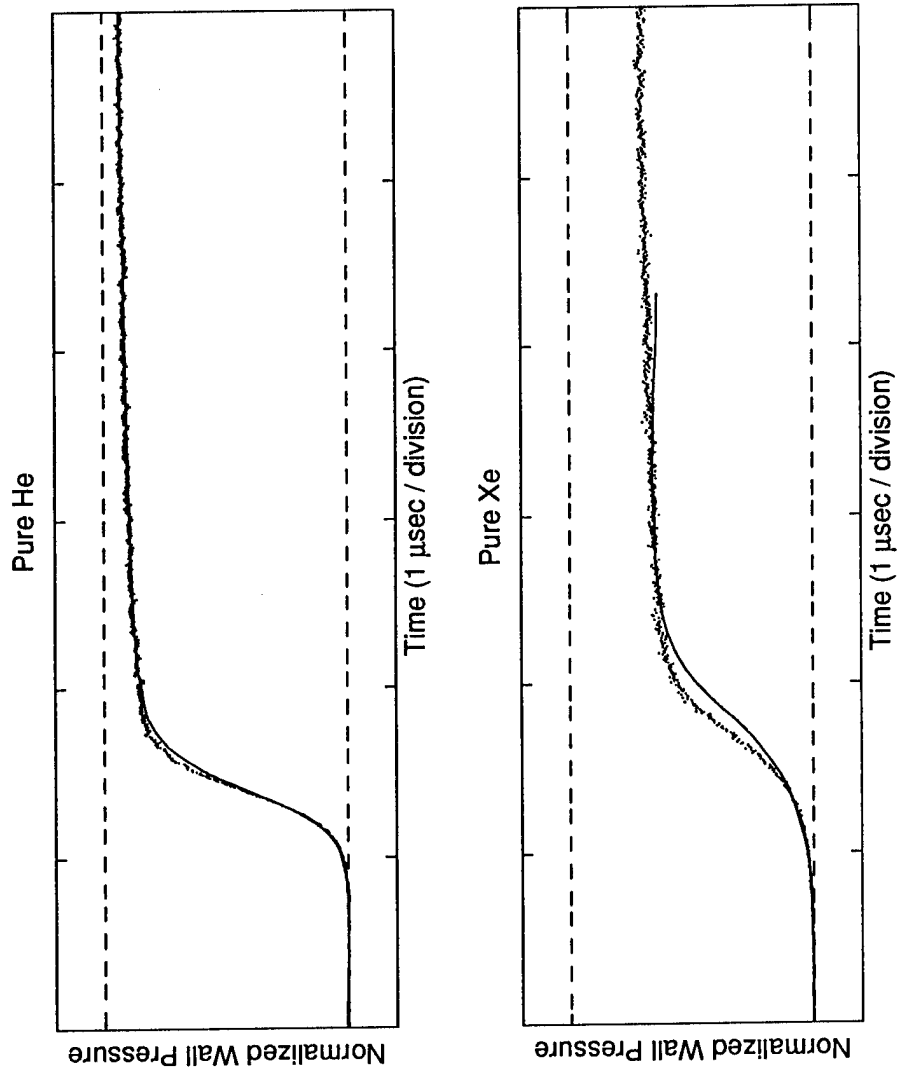
14

Figure 3. Time traces of the wall pressure for pure He and pure Xe flows. The solid line denotes experimental data while the dotted line represents the simulated profile.
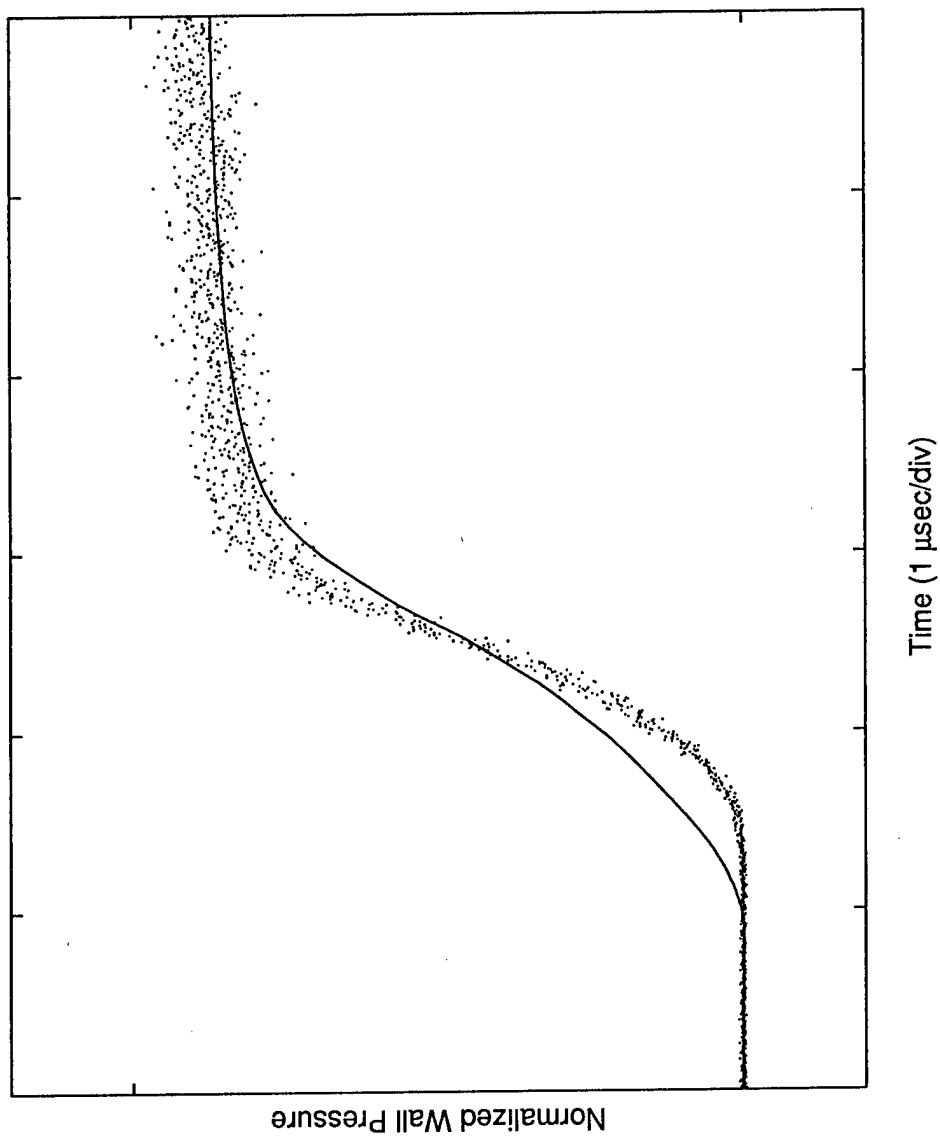
Figure 4. Time trace of the wall pressure in a 92.3% He - 7.7% Xe flow. The solid line is the experimental data and the dotted line is the simulated profile. The simulated result was obtained using Chapman and Cowling data for the like-species collision parameters and the arithmetic mean combining rule for the inter-species values.
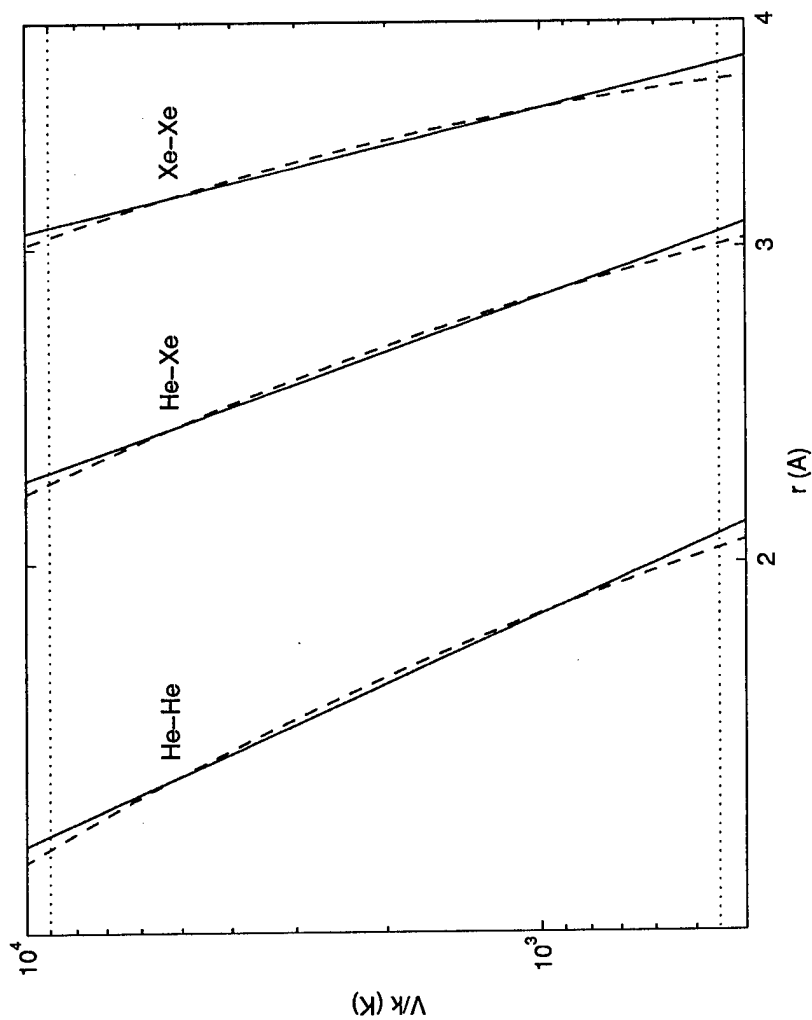
16

Figure 5. Intermolecular potentials for the three classes of collisions that take place in a binary mixture of He and Xe. The dashed lines are the HFD-B potential and the solid lines are power-law curve fits. The potentials are displayed over the temperature range of interest.
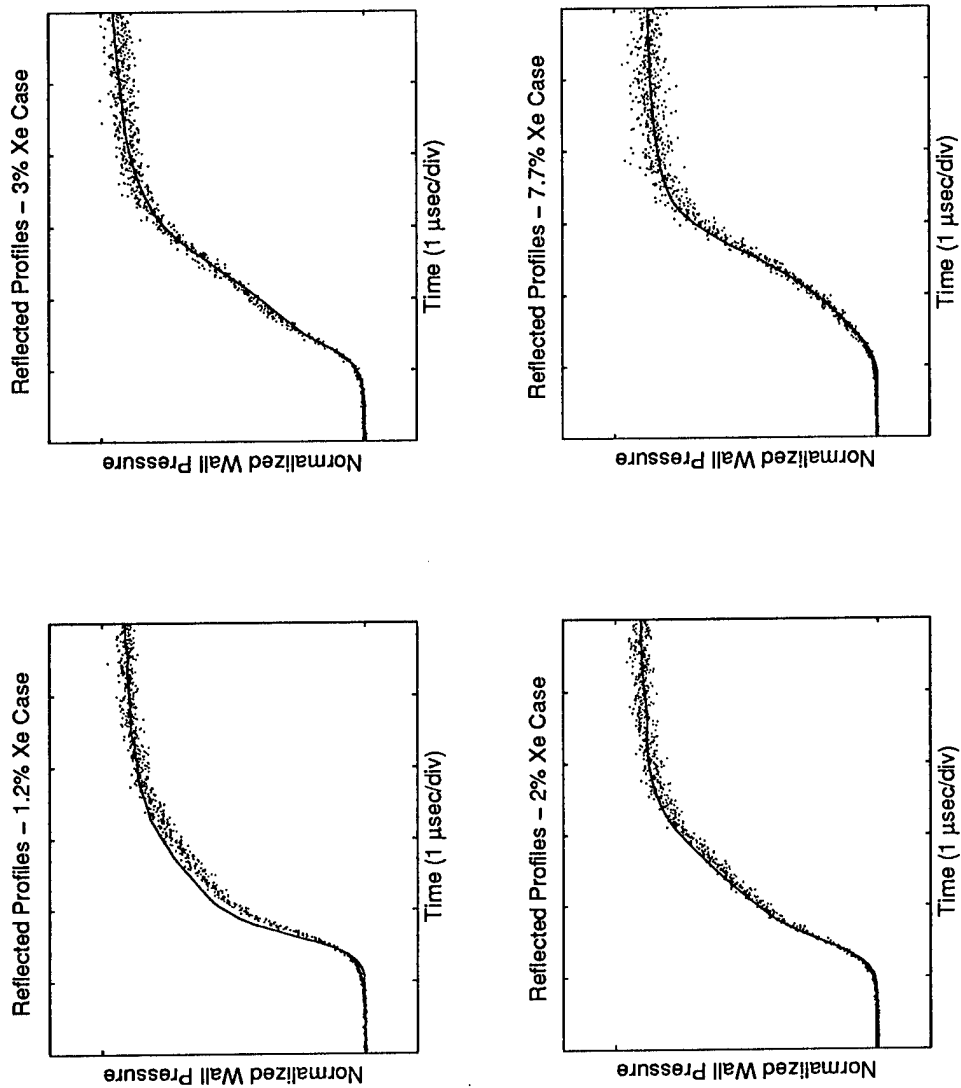
Figure 6. Time traces of the wall pressure for several concentrations of Xe. The solid line is the experimental data and the dotted line is the simulated profile.
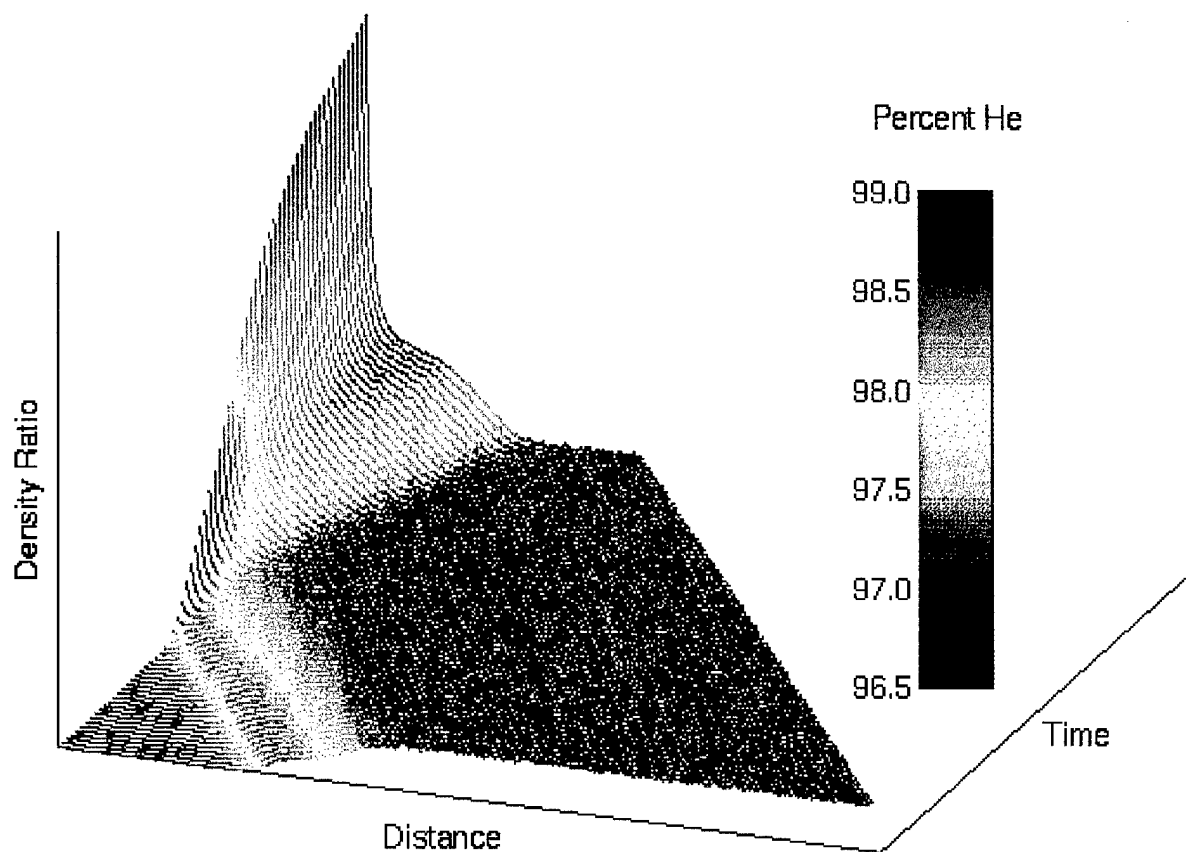
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Figure 7. Mass averaged mixture density resulting from the reflection of a shock wave in a 97% He - 3% Xe mixture from a cold wall. The color scale corresponds to the local He concentration.
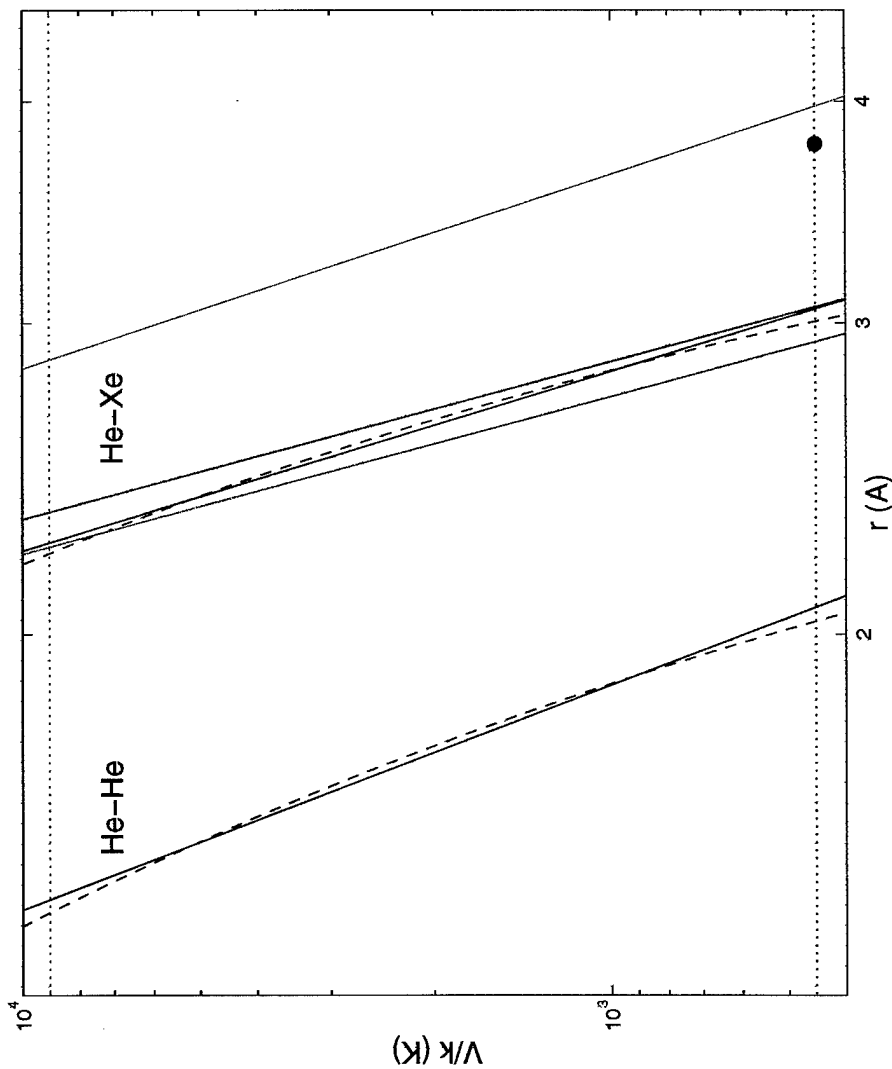
Figure 8. Intermolecular potentials for the three classes of collisions in a mixture of He and Xe. The black lines correspond to the HFD-B potential. The green line is the arithmetic average of the HFD-B data and the red line is the geometric mean combining rule. The light blue line is the arithmetic average of the Chapman and Cowling data. The black-dot is the Xe-Xe reference diameter from the HFD-B power-law fit.
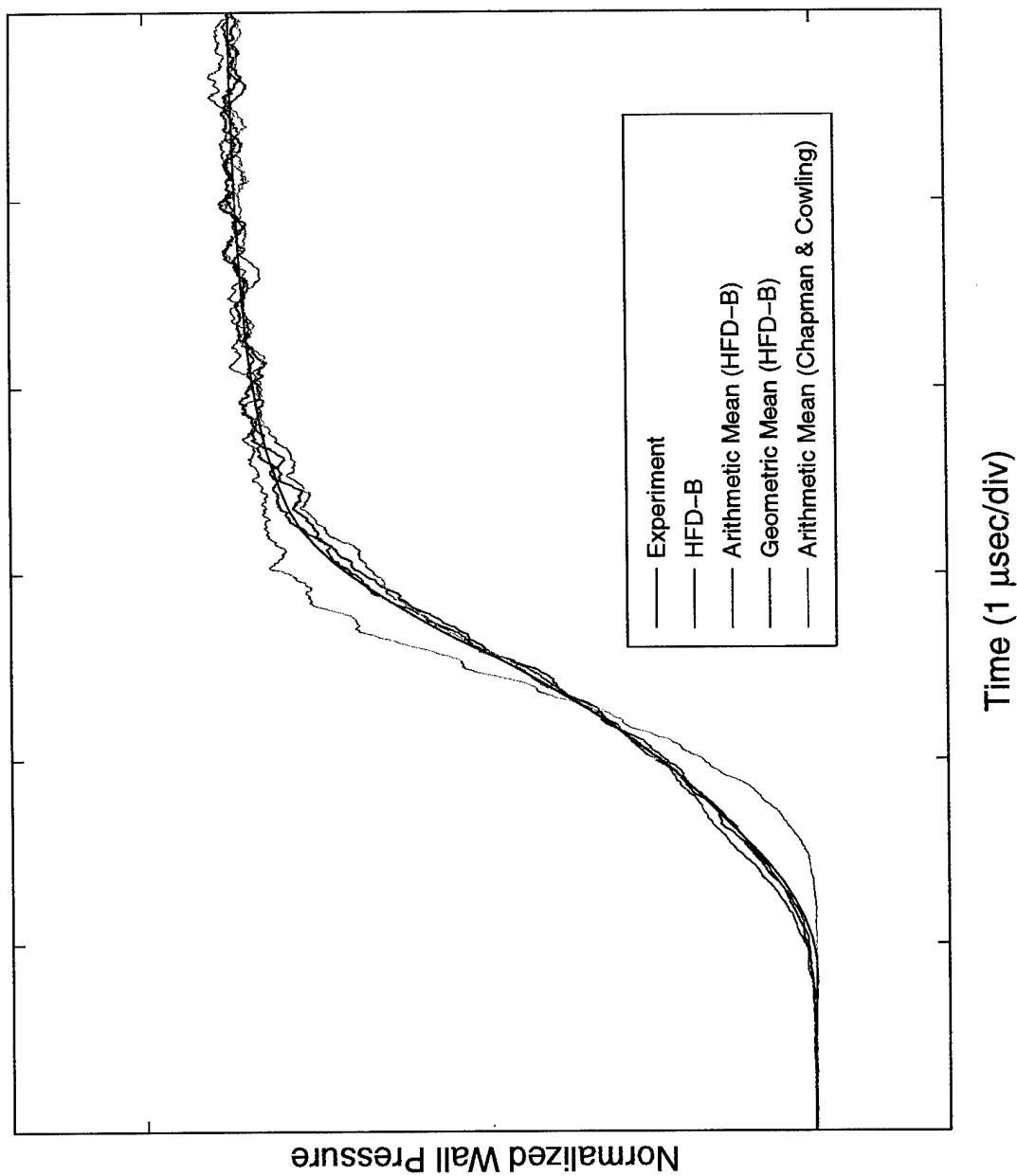
Figure 9. Time trace of the wall pressure in a 92.3% He - 7.7% Xe flow using various combining rules and potentials.

The plot legend reads:
- Experiment
- HFD-B
- Arithmetic Mean (HFD-B)
- Geometric Mean (HFD-B)
- Arithmetic Mean (Chapman & Cowling)

Axis labels:
- Normalized Wall Pressure
- Time (1 μsec/div)